Nanoscience for Insensitive Munitions Development

Presentation for Topical Panel

Nano and Biological Technology and Their Potential Applications

December 3, 2008

Presented by:

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Aberdeen Proving Ground, MD 21005

Report Documentation Page

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Goals:

Approach:

- Develop predictive capability
- Identify fundamental reaction mechanisms
- Assess and advance methods and models

- Quantum Mechanics
- Classical Molecular Dynamics
- Empirical Methods

Benefit to the Warfighter:

- Increased Lethality
- Reduced vulnerability
- Faster, cheaper

Expanding ARL mission efforts

IHEM01A/Theoretical Characterization of Energetic Materials

Develop enabling technologies to predict chemical and physical properties of EM to make *a priori* assessment of performance and vulnerability

US Army Research, Development and Engineering Command Environmental Quality Technology Ordnance Program "Design and Formulation of Novel Energetic Material Replacements for RDX"

Replace RDX with EM ingredients that have:

- Reduced toxicity, reduced hazard combustion/detonation products
- Equivalent performance properties
- Meet and/or exceed JROC 113-04 Insensitive Munition (IM) compliance requirements.

Office of Naval Research "Energetic Materials Modeling & Simulation Tools"

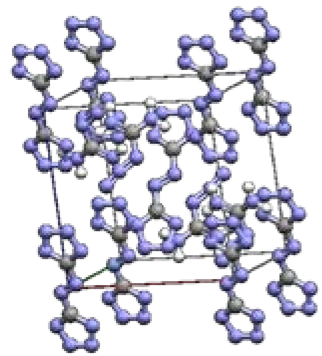
Assess and evaluate emerging models and software for EM research

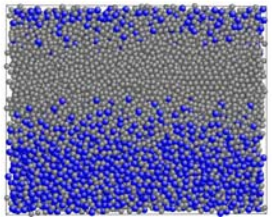
HSAI for Multi-Scale Reactive Modeling and Simulation of Insensitive Munitions

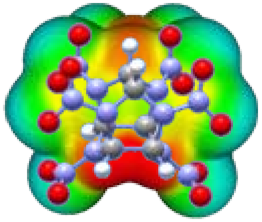
Collaborators and contributors

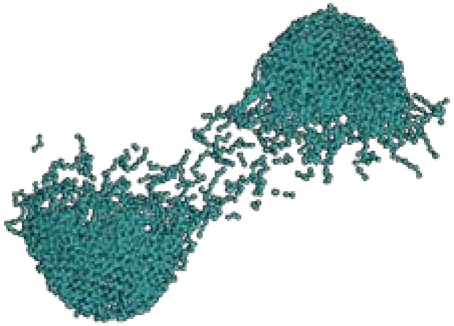
ARL

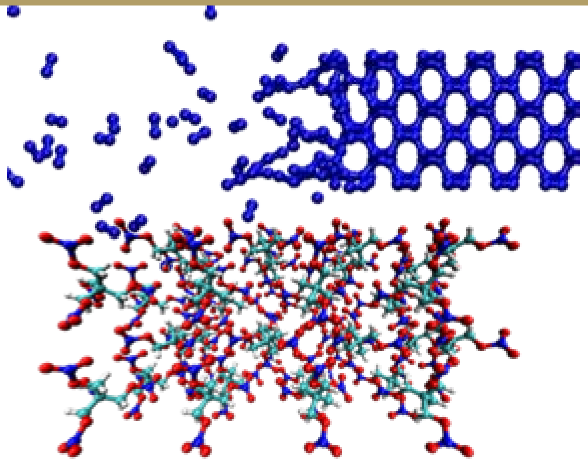
Edward F. C. Byrd
John K. Brennan
William D. Mattson
Jennifer Ciezak
Rad Balu
Scott Weingarten
Anthony Yau

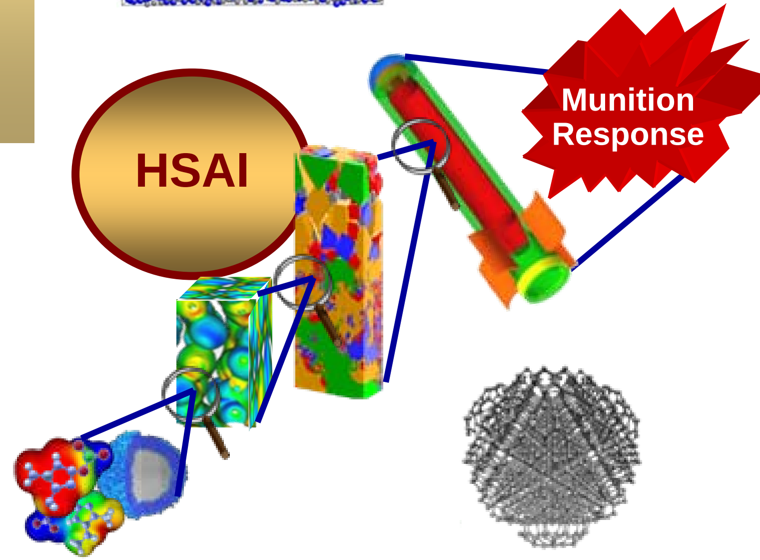










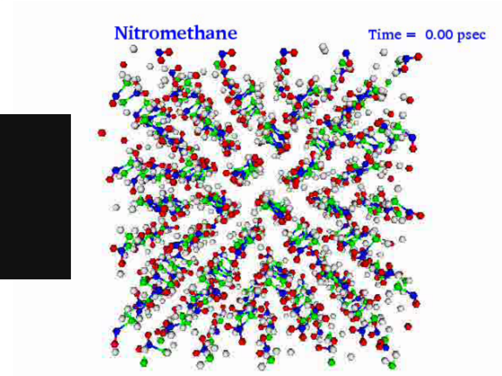


Ludwig Maximilians Universität München LMU
North Carolina A&T State University explore. discover. become.
Rutgers The State University of New Jersey
Washington State University World Class. Face to Face.
Rice Unconventional Wisdom
Department of the Navy ONR Science & Technology
NAVSEA Indian Head Surface Warfare Center Division
Caltech
Maryland Terrapins
Mizzou University of Missouri
University of Minnesota
Sandia National Laboratories
HPTi
Johns Hopkins University
DoD HPC Modernization Program
Los Alamos National Laboratory
Stone Ridge Technology
NC State
Alabama A&M University
US Army RDEC CECOM Fort Monmouth Bottom Line The Soldier
University of Delaware
NETL National Energy Technology Laboratory
Lawrence Livermore National Laboratory Science in the National Interest

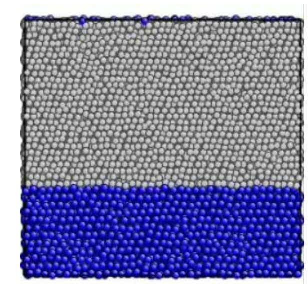
Simulations used to explore dynamical behavior

Classical MD

Self-sustained detonation of model explosive



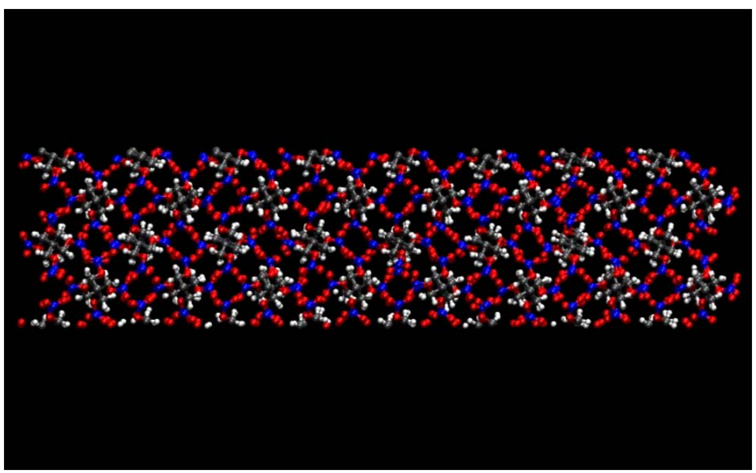
Melting of nitromethane



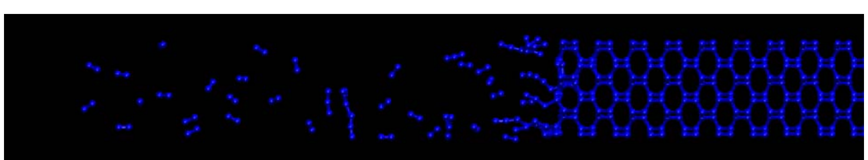
Thermal initiation of reactive material Ni/Al

Quantum MD

Shocked energetic materials

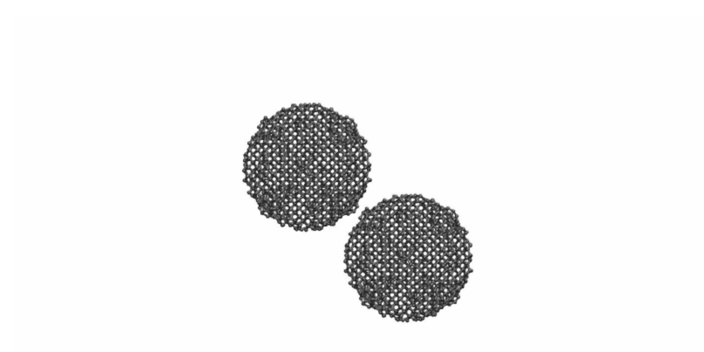


Conventional



Disruptive

Hypervelocity collisions of ND



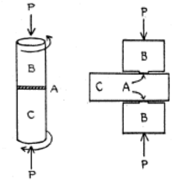
Exploring Structural Bond Energy Release (SBER) in Nano-Diamonds using Quantum Molecular Dynamics and Static High Pressure

William D. Mattson, Radhakrishnan Balu, Betsy M. Rice, and Jennifer A. Ciezak

SBER: The release of excess energy stored in chemical bonds from structurally deformation by compressing, stretching or twisting the bond.

First Observed by Bridgeman as Explosion of Common Substances Subjected to Pressure and Shear

Effects of High Shearing Stress Combined with Hydrostatic Pressure



Physical Review, 48 (1935) 825-47

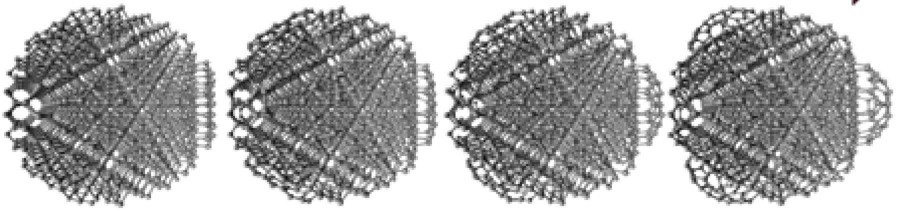
Former Soviet Union had Extensive SBER Program, with Particular Interest in Diamond

Structural Bond Energy Release in Energetic Materials as New Means for Designing Nonconventional High Explosives: An analysis of Soviet Research, Tech Report 1991. A. M. Al'tschuler, Technical Report TRC-91-0003, Technical Research Corporation, McLean, VA (1991).

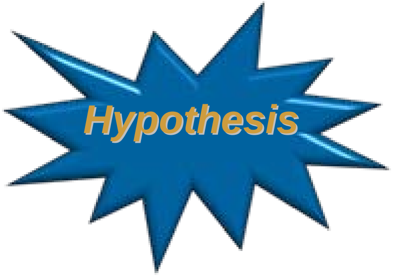
Potential Structural Bond Energy Materials

✓Polymeric Nitrogen, an Extended Solid 8xTNT
✓Nano-Diamonds, a Nanometer Scale Cluster 5xTNT

QM Diamond Surface Reconstruction with Buckyball Features



- Quantum simulations of smaller ND clusters show surface reconstruction to fullerene arrangement, core maintains diamond structure
- Calculations show tensile stress on the surface. Our calculations suggest core pressure in excess of 50GPa.



Sudden Disruption of ND Surface will Release Energy Stored in the Compressed Core

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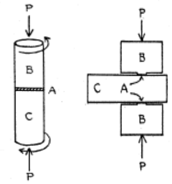

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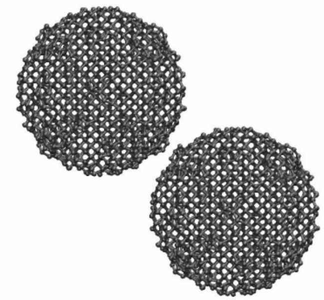


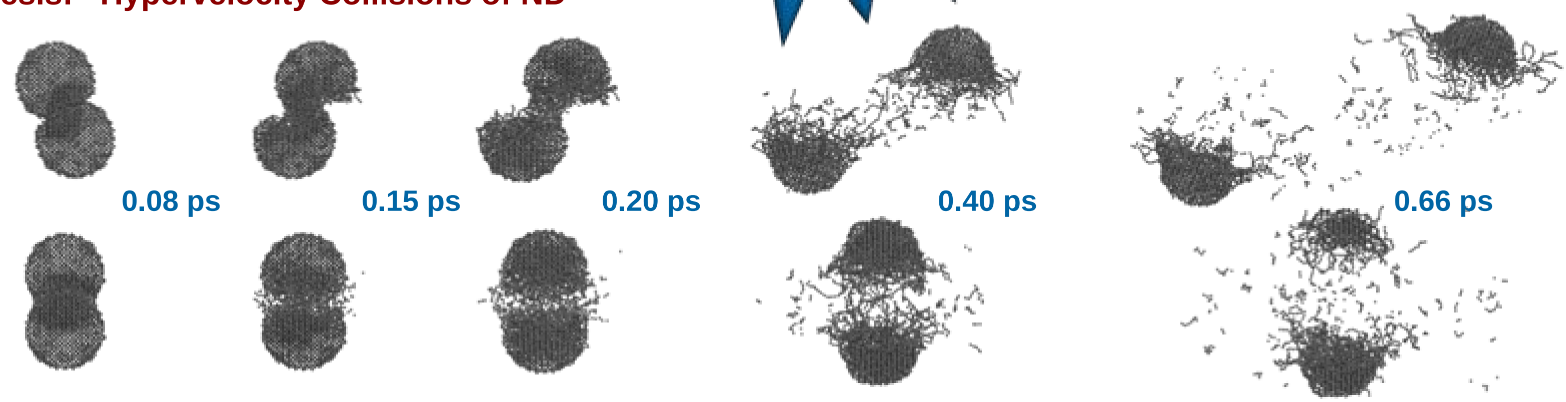
Hypothesis

Sudden Disruption of ND Surface will Release Energy Stored in the Compressed Core

Testing the Hypothesis: Hypervelocity Collisions of ND

Perpendicular to Axis of Collision

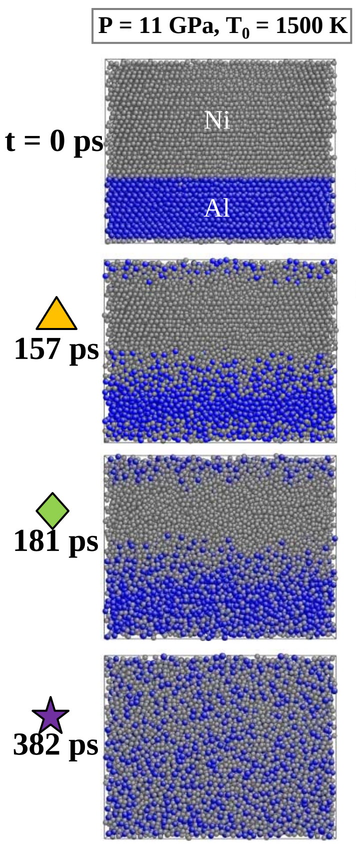
Along Axis of Collision

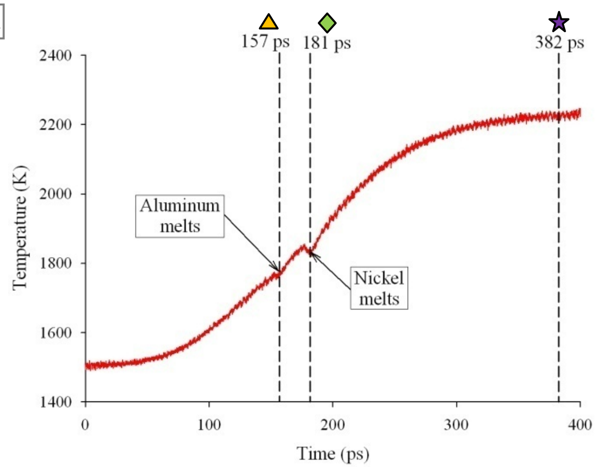


Identifying the Role of Pressure on the Response of Reactive Material to Thermal Initiation: A Molecular Dynamics Study

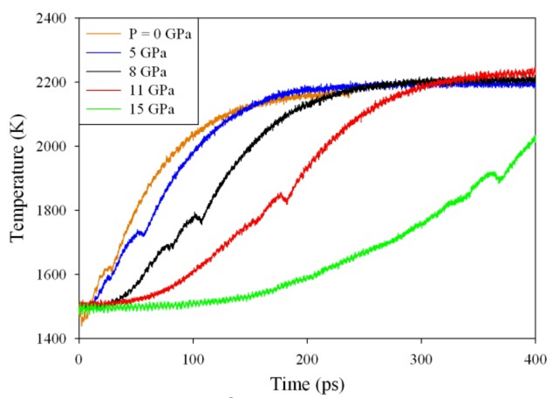
N. Scott Weingarten, William D. Mattson, Anthony D. Yau, and Betsy M. Rice (ARL) and Timothy P. Weihs, The Johns Hopkins University

Molecular dynamics (MD) simulations in the NPH ensemble (number of particles, pressure and enthalpy held constant):





Pressure strongly influences rate of alloying



- **Curves have same features: two "kinks" that correspond to melting of the two layers.**
- **Al melting always precedes Ni melting**
- **With increase in pressure, point of Al melting is less distinct**

Tempe

- Initial NVE-MD simulations at T=1100K, reactions were quenched, in disagreement with experiment
- Heating produced by reaction caused significant internal pressure which quenched the reactions
- NPH-MD simulations eliminate this problem: reaction rates are strongly influenced by imposed pressure.

TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.

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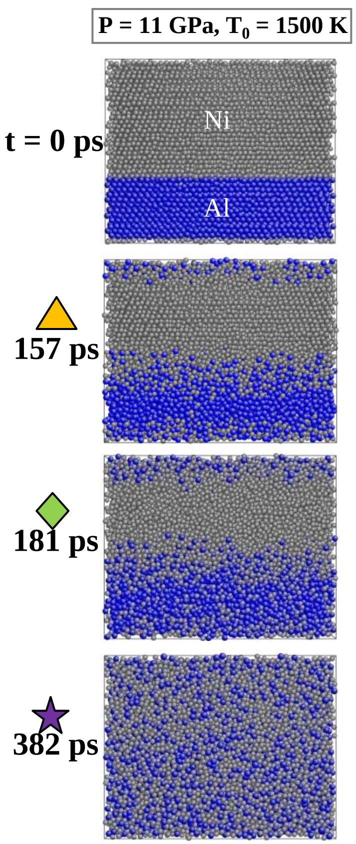

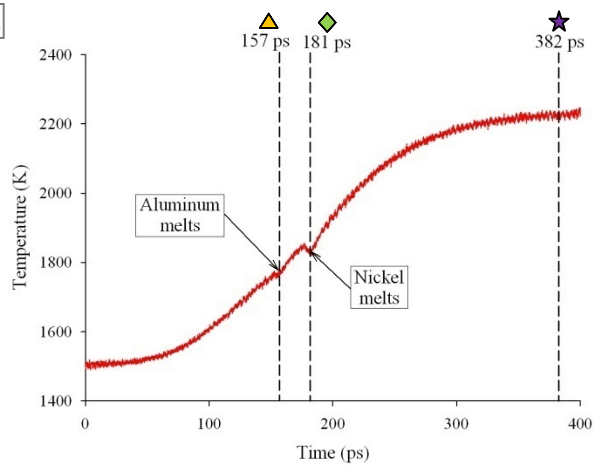

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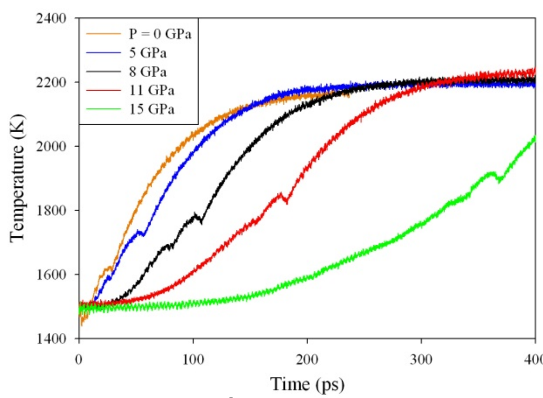

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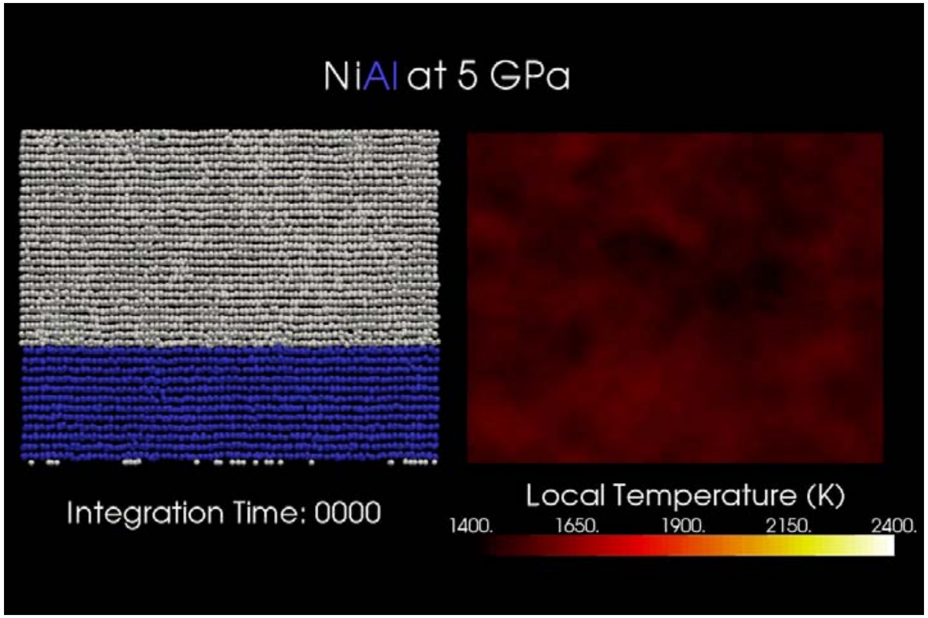
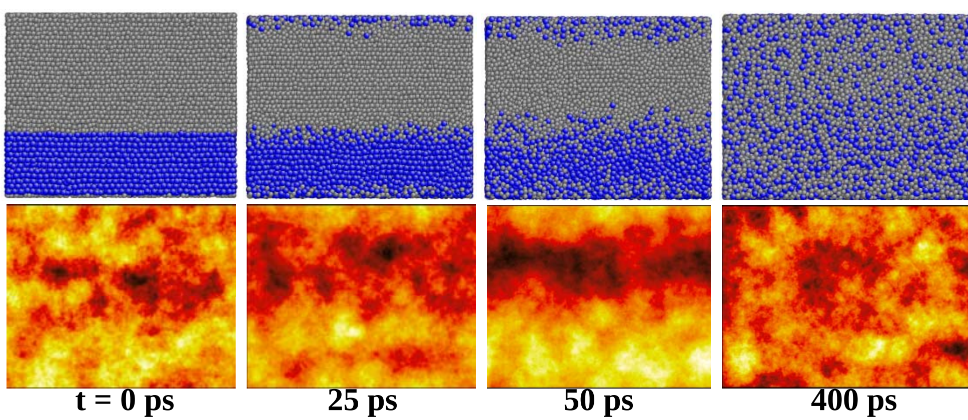


Temperature inhomogeneities in reacting bilayer:



TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.

Transitions to:

Experimental Programs:

- Assist in experimental data interpretation
- Explore phenomena at inaccessible scales
- Validate or remedy models and methods

ONR

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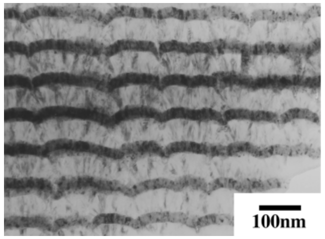
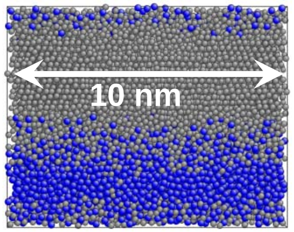
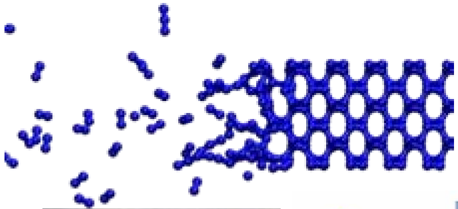


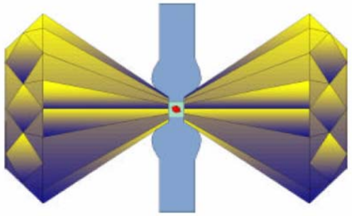


Nanolaminates of reactive materials



Polynitrogen

35 GPa



CDAC

Theoretical Programs:

High Performance Computing Software Application Institute for Multi-Scale Reactive Modeling and Simulation of Insensitive Munitions

ARL DoD HPC Modernization Program

New Six-Year Program

Questions?